ATOMIC SCALING PROCESSES DURING BRITTLE FRACTURE

Final Report

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The goals of this research was to understand the relationship between bond rupture and macroscopic features on the fracture surface and to determine the effect of microstructure on fracture processes. Toward this goal three papers were written, one more is planned and five presentations were made.

Several important findings were discovered during the course of the project. These findings include the determination that fracture in single crystals on the same fracture plane but stressed in different directions have different toughness values,different fracture morphology and different fractal dimensions, that the characteristic atomic parameter, a_0, appears to be equal to the bond distances in fracture, that the profile dimension is not equal to the contour dimension when determining the fracture surface (fractal) dimension and that the fractal dimensional increment is equal to the crack size-to-(mirror-mist) branching boundary ratio [flaw-to-mirror size ratio]. For the sake of discussion, these results will be discussed in the following categories: Effects of Microstructure on Fracture, Effect of Bond Type on Fracture, Particle Emissions During Fracture and Analytical Models.

Effects of Microstructure on Fracture

1. Single Crystal Fracture - The main part of the experimental effort was spent on studying the fracture of single crystal silicon. From this study, several important discoveries were made. These discoveries include the determination that fracture in single crystals on the same fracture plane but stressed in different directions have different toughness values, different fracture morphology and different fractal dimensions, that the characteristic atomic parameter, a_0, appears to be equal to the bond distances in fracture, and that the fractal dimensional increment is equal to the crack size-to-(mirror-mist) branching boundary ratio [flaw-to-mirror size ratio]. These findings will be discussed individually below.

Fracture of single crystal silicon was undertaken to determine the effect of stressing direction on the fracture morphology and resistance to fracture without the interference of microstructure. Since previous studies outlined the fracture in silicon, this study concentrated on fracture in the (110) plane with the stress applied in the [100] or [110] directions. The fracture toughness in the [100] direction was 1.23 ± 0.09 $MPam^{1/2}$ with a corresponding fractal dimensional increment of 0.10 ± 0.04 and in the [110] direction the fracture toughness was 1.07 ± 0.09 $MPam^{1/2}$ with a corresponding fractal dimensional increment of 0.04 ± 0.03. The fracture surface appeared quite different in the two stressing directions. In previous work, we showed that the fracture energy, g, can be related to the fractal dimensional increment, D*: $\gamma = (1/2)\, E\, a_0\, D^*$ where E is the elastic modulus and a_0 is an atomic characteristic parameter. In this case, E is taken in the stressing direction for the single crystal and a_0 was calculated to be 8.35 Å and 9.76 Å corresponding to the [110] and[100] directions, respectively. The lattice parameter length is 5.43 Å and the unit cell diagonal length is 9.41 Å. Thus, the characteristic length is about the same length as the diamond cubic unit cell. We conclude that the Si-Si diagonal bond is the basis of the elementary fracture process in Si on the (110) plane. A measurement of the fractal dimension was made on single crystal silicon using the scanning tunneling microscope by Bonnell at the University of Pennsylvania. The fractal dimensional increment was found to be 0.07 in reasonable agreement with the present study. Note that the fracture plane for the latter measurement was (111) and not (110) so that differences would be expected.

When brittle materials fracture, three approximately symmetric, characteristic regions appear on the fracture surface surrounding the fracture initiating crack. These regions have become known as mirror, mist, and hackle. The distances between the fracture initiating crack and the demarcations between the regions are related to the stress at failure and have been collectively called the fracture mirror regions. These features are precursors to crack branching and end on one plane at the point of macroscopic crack branching. However, after branching, the features will repeat and branch again and again, if there is enough material. Previous research determined that the flaw to mirror size ratios are constant in fast fracture. Recent research under this contract has shown that the flaw size to (mirror-mist) size ratio constant is equal to the fractal dimensional increment. This fact can be demonstrated experimentally and theoretically. Theoretically we can show that the two quantities have to be related to each other if two separately observed experimental relationships are valid. It has been observed experimentally that K_{IC} is proportional to the fractal dimensional increment, D*, and that K_{IBj} is proportional to the elastic modulus, E. We can represent these relationships as follows:

$$K_{IC} = E\,(a_0\,D^*)^{1/2} = Y(\Theta)\,\sigma_f\,c^{1/2} \qquad (5)$$

and

$$K_{IBj} = b_0{}^{1/2}\,E = Y(\Theta)\,\sigma_f\,r_j{}^{1/2} \qquad (6)$$

where K_{IBj} is a critical value of the branching stress intensity (j = 1,2 & 3 corresponding to the mirror-mist, mist-hackle and macroscopic crack branching boundary), b_0 is a characteristic distance on the atomic scale, Y(Q) is a crack border correction factor, c is the radius of a semi-circular flaw, σ_f is the fracture stress, r_j is the radius from the origin of fracture to each of three boundaries (j = 1,2,3), and the other terms have been previously defined. The right hand sides of equations (5) and (6) are based on existing fracture mechanics analyses. If we assume that a0 is proportional to b0, then the flaw-to-mirror size ratio is proportional to D*. Further, notice that if $b_0 = a_0$, then for j = 1,

$$c/r_j = D^* \qquad (7)$$

Experimentally the two quantities in Eq. (7) have been compared for PZT, Si, Pyroceram 9606, alumina, ZnS and ZnSe in Table 1. Notice that the values compare quite well. The implications of this fact are that the fracture features are self-similar, the appearance of these (macroscopic) features are related to the atomic structure (fractal dimensional increment to Si bond length) and that the structure on the macroscopic and atomic scale can be related quantitatively to the fracture process.

2. Effect of Grain Size on Fracture - We examined the fracture of ZnS bars with different grain sizes, i.e. about 5 μm and 100 μm average grain size material. The calculation of fracture toughness (K_{IC}) of these materials was directly related to the crack size to grain size ratio. The grain size was that measured at the point of failure and not the average grain size. If the crack was contained in a large grain, the fracture resistance was equal to that of a single crystal whereas if the crack was larger than about 10 grains, the fracture resistance was equal to a polycrystalline value. The polycrystalline value of fracture toughness (K_{IC}) is about 3 times larger than the single crystal value. The fractal dimension of the fracture surfaces from the same specimens increase with the increase in crack size-to-grain size ratio in the identical manner as the fracture toughness. There is a one-to-one correspondence for each specimen as shown in Figure 2. In addition, measurements of the fractal dimension using measuring units above and below the grain size resulted in the same measurement. The

combined behavior described above implies that the resistance to fracture and the tortuosity of the crack surface for materials that are cubic and have no other mechanism than grain deflection for toughening is determined during the initiation of fracture and governed by the atomic bonding and not by the microstructure, i.e. grain size. Thus, the most effective toughening scheme for these materials should be performed at the atomic level.

Effect of Bond Type on Fracture

The fractal dimensions were measured on several single crystals in order to understand the relationship of bond type on fracture. D* was obtained on calcium fluoride (0.07), silicon (0.04-0.1), alumina (0.19) , and a spinel [$MgAl_2O_4$] (0.09). Even though there was a range in ionicity from almost completely ionic (CaF_2) to completely covalent (Si), there was no obvious difference in behavior in terms of the fractal dimension. Also, there was no obvious correlation to structure type, e.g., cubic vs. spinel. However, several observations are important. In all cases examined, the fractal dimension of the single crystal was slightly lower than the polycrystalline material with the same structure. Thus, the single crystal appears to be a "lower bound" fractal dimension for that structure. Microstructural features, i.e., grain boundaries, pores, inclusions, etc., add to the tortuosity. However, it appears that these features do not add a significant amount to the dimensionality. This fact combined with the observations indicated above, i.e., the flaw-to-mirror size ratio is proportional to the fractal dimensional increment, the measurement of D* above and below the grain size in ZnS and that D* varies with fracture plane and direction, leads to the conclusion that the tortuosity on the fracture surface is produced by the fracture process and is more related to the strength of atomic bonds and not the microstructural features. However, the materials selected for study do not have intentionally added microstructural features to provide added toughening. Thus, the above statement does not preclude another mechanism to change the tortuosity, e.g. transformation toughening or second phase additions may affect the fracture process and the fracture morphology.

Particle Emissions During Fracture

Professor J. T. Dickinson and his co-workers at Washington State University have discussed their research with us. As a result of this dialog, they were able to measure the fractal dimension of MgO from the slope of the amplitude - frequency curve of the light emitted during fracture. These initial results appears to indicate that the intensity of light emitted

during fracture is fractally distributed in time. The fractal dimension obtained in this manner is in reasonable agreement with that obtained using more conventional techniques.Photons would be expected to be fractally distributed if they were being emitted from a fractal surface. This finding provides a means by which we can compare atomic processes (photon emission) with macroscopic observations (fracture topography) and relate these through fractal analysis.

Analytical Modelling

1. Finite Element Modelling - Ideal fractal fracture surfaces were generated using a computer generated mid-point displacement algorithm. From these generated surfaces, important conclusions were made regarding the measurement of fractal dimensions. Dimensions determined from profiles of the fracture surface are not always equal to the true dimension, whereas the contour dimensions, i.e., dimensions determined from planes approximately parallel to the fracture surface provide quite reasonable estimates of the true surface dimension. In addition polishing angles of up to 40° from the horizontal are permissible for accurate measurements. These exercises were necessary to establish the proper techniques and mathematically verify their correctness.

2. Closed Form Solutions - The relationship between the fracture energy, γ, and the fractal dimensional increment, D^*, is still a useful equation:

$$\gamma = 1/2\ (E\ a_0\ D^*) \qquad (8)$$

This equation can be used to relate the fracture surface energy, γ_s, i.e. the single crystal value of resistance to fracture, to the fracture energy of the polycrystalline material, γ_f:

$$\gamma_f\ /\ \gamma_s = (\pi^2/2)(E_f/E_s)a_0 d_0\ D^*/\ a^2 \qquad (9)$$

where E_f and E_s are the elastic moduli of the polycrystalline and single crystal material respectively, d_0 is the crystal lattice spacing and a is the atomic radius. Reasonable agreement has been found between the predicted and observed fracture energy ratios [Eq. (9)] with the limited number of materials examined so far.

3. Fractal-Griffith Equation - As part of this program an attempt at modelling fracture as a fractal process resulted in the derivation of the Fractal - Griffith equation. This involves an energy balance approach which incorporates a fractal, i.e. non-Euclidean, crack. The result is :

$$\gamma_f = \pi\sigma^2 c/\ (2E)[(1/D)\ (c/a_0)]^{1-D} \qquad (10)$$

where c is the critical crack size, D is the fractal dimension ($1 < D < 2$), and the other terms are as previously defined. For a fractal dimension of 1, i.e., for an Euclidean crack, the above expression reduces to the conventional Griffith expression. More importantly, if we rearrange the expression [Eq. (10)] with the relationship that $\sigma = E\ \varepsilon$, where ε is the critical strain at failure, then Eq. (10) can be expressed in the form of Eq. (8). It is very encouraging that we now can demonstrate a relationship between experimental data (Eq. (8) is based on experimental data) and a theoretically derived expression for fracture energy which allows for a fractal shaped crack.